

6«alpha»-Hydroxy-4-Chloro-1,2,dehydro-17«alpha»-methyltestosterone-tris-TMS

InChI: InChI=1S/C29H51ClO3Si3/c1-27-16-15-23(31-34(4,5)6)26(30)25(27)24(32-35(7,8)9)19-2
InChIKey: RJRDWQNBTOPZNE-UHFFFAOYSA-N
Formula: C29H51ClO3Si3
SMILES: CC12C=CC(O[Si](C)(C)C)=C(Cl)C1=C(O[Si](C)(C)C)CC1C2CCC2(C)C1CCC2(C)O[Si](C)(C)C
Mol. weight [g/mol]: 567.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.06		Crippen Method
logp	9.426		Crippen Method
rinpol	3018.00		NIST Webbook
rinpol	3018.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U412281&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/74-643-6/6-alpha-Hydroxy-4-Chloro-1-2-dehydro-17-alpha-methyltestosterone-tris-TMS>

Generated by Cheméo on 2024-04-20 12:55:30.511406574 +0000 UTC m=+15906979.431983889.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.